PARTISN — Introduction and System Overview

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INTRODUCTION

This document is the central user methods and programming documentation for PARTISN. PARTISN is an acronym for PARallel, TIme-dependent SN.

The PARTISN code package is a modular computer program package designed to solve the time-independent or dependent multigroup discrete ordinates form of the Boltzmann transport equation in several different geometries. The modular construction of the package separates the input processing, the transport equation solving, and the post processing (or edit) functions into distinct code modules: the Input Module, the Solver Module, and the Edit Module, respectively. PARTISN is the evolutionary successor to the DANTSYS^{TM} code system package. The Input and Edit Modules in PARTISN are very similar to those in DANTSYS. However, unlike DANTSYS, the Solver Module in PARTISN contains one, two, and three-dimensional solvers in a single module. In addition to the diamond-differencing method, the Solver Module also has Adaptive Weighted Diamond-Differencing (AWDD), Linear Discontinuous (LD), and Exponential Discontinuous (ED) spatial differencing methods. The spatial mesh may consist of either a standard orthogonal mesh or a block adaptive orthogonal mesh. The Solver Module may be run in parallel for two and three dimensional problems.

Some of the major features included in the PARTISN code package are:

- a free-field format ASCII text input capability;
- the use of a diffusion or transport synthetic acceleration scheme to accelerate the iterative process in the Solver Module;
- direct (forward) or adjoint calculational capability;
- standard plane, two-angle plane, cylindrical or spherical geometry options for 1-d;
- x-y, r-z and r-theta geometries in 2-d;
- x-y-z and r-z-theta geometries in 3-d;
- arbitrary anisotropic scattering order;
- vacuum, reflective, periodic, white, or surface source boundary condition options;
- inhomogeneous (fixed) source or k_{eff} calculation options as well as time-absorption (alpha), nuclide concentration, or dimensional search options for time-independent calculations;
- time-dependent calculations with time-dependent sources and/or cross sections;

- a variety of spatial differencing methods;
- a ray trace first collision option to obtain a first collision source from an arbitrary source distribution;
- a strictly positive scattering source option;
- an automatic mesh coarsening option;
- user flexibility in using both ASCII text or sequential file input;
- user flexibility in controlling the execution of both modules and submodules;
- extensive, user-oriented error diagnostics.

PARTISN is a large, very flexible code package. Great effort has been devoted to making the code highly user-oriented. Simple problems can be easily run and many of the code options can be ignored by the casual user. At the same time numerous options for selective and sophisticated executions are available to the more advanced user. In all cases, redundancy of input has been minimized, and reasonable default values for many input parameters are provided. The input is designed to be meaningful, easily understood, easily verified, easy to change, and logically common. The printed output is well documented with liberal use of descriptive comments and headings.

DOCUMENTATION SUMMARY

The S_n Code package includes documentation for varying audiences.

Table 1.1 Documentation Elements

Documentation Type	Title
Methods	Methods Document
Introduction	Introduction and System Overview
User's Guide	PARTISN User's Guide
Details	Details of the Geometry and Solver Input
Details	Running the Edit Module
Reference	Free Field Input Reference
Reference	Cross Section Libraries
Details	Material Mixing Tutorial
Methods	Methods Document
Details	Code Structure
Reference	Error Messages
Reference	File Descriptions
Reference	Solver Module Abstracts
Reference	Bibliography

As in the case of PARTISN, this manual has evolved from the DANTSYS manual (Ref. 1). It contains all of the DANTSYS documentation (excepting the User's Guides), but with expanded sections where necessary to cover the new capabilities in PARTISN.

COMMON MODELING CONCEPTS

Geometry Concepts

In the specification of geometry and space-variable related input, the user must be familiar with the nomenclature used by PARTISN. The terms fine mesh, coarse mesh, and zones are defined below for the orthogonal geometry mesh used in PARTISN.

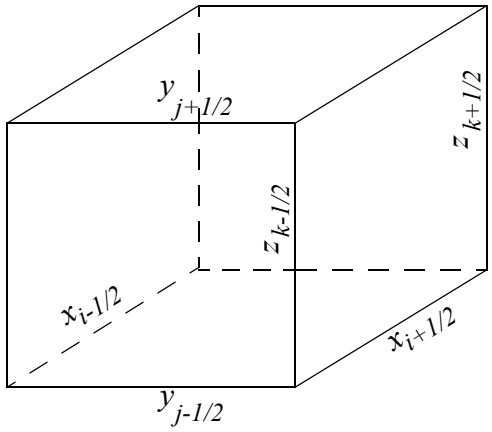

Figure 1.1 Spatial mesh labeling convention in PARTISN.

The fine mesh is the spatial solution-mesh for the problem, as depicted in Figure 1.1 above. Each fine mesh, or fine mesh interval, is bounded by an adjacent pair of fine-mesh grid-surfaces $x_{i-1/2}$ and $x_{i+1/2}$ with $x_{i-1/2} < x_{i+1/2}$ in the x direction; $y_{j-1/2}$ and $y_{j+1/2}$ with $y_{j-1/2} < y_{j+1/2}$ in the y direction; $z_{k-1/2}$ and $z_{k+1/2}$ with $z_{k-1/2} < z_{k+1/2}$ in the z direction There are IT, JT and KT such fine mesh intervals respectively. No material discontinuities may occur within a fine mesh interval. The specification of the fine mesh is accomplished by specifying how many equally sized fine mesh intervals there are in each coarse mesh.

The coarse mesh is a spatial superset of the fine mesh and is formed by partitioning the spatial domain of the problem into a suitable number of “coarse” intervals. There are IM, JM, and KM coarse mesh intervals in each of the coordinate directions spanning the problem. Each coarse mesh interval contains one or more fine mesh intervals. All fine

mesh intervals within a coarse mesh interval have equal widths. No material discontinuities may occur within a coarse mesh interval.

The zone is a spatial superset of coarse mesh intervals and is characterized by a single set of multigroup nuclear properties, i.e., cross sections, so that all fine mesh intervals within a zone have the same cross sections. The user assigns a zone number to each coarse mesh interval. The zone number tells the code which macroscopic cross section set is to be used within that zone. Coarse mesh intervals having the same zone number need not be simply connected.

A zone number of 0 (zero) can be used to specify that a coarse mesh interval is a pure void (all cross sections are identically zero).

In the block adaptive mesh, the coarse meshes define the block structure. Then, within each individual block (coarse mesh), an arbitrary level of coarsening is applied to that block's fine mesh, resulting in a block adaptive mesh structure. This structure is used only within the Solver Module; the Input and Edit Modules see only the user-input coarse/fine (single level) mesh.

More detail on these concepts is to be found on page 3-15.

Iteration Strategy

In this section is described the basic iteration strategy used in the execution of the Solver Module. A more detailed description of the strategy is given on page 3-17 including the iteration controls that the user inputs and a discussion of the iteration monitor printout that is printed in the output.

The basic features of the iteration strategy are shown in the simplified flow diagram in Figure 1.2.

The iterative strategy is basically divided into three parts: inner iterations, outer iterations, and eigenvalue search iterations.

The inner iterations are concerned with the convergence of the pointwise scalar fluxes in each group due to iteration on within-group scattering processes. For eigenvalue problems, the source to each group is given by the fission source from the previous outer iteration plus any in-scattering sources. For fixed source problems, the source to each group is the input source distribution plus the in-scattering source.

The outer iterations are concerned with the convergence of the eigenvalue, the fission source distribution and the energy-group upscatter source if any or all are present.

The eigenvalue search iteration is the ability of the code to adjust some parameters of the problem, namely the isotopic concentrations or the spatial dimensions of selected coarse mesh intervals, to obtain a desired value of the k_{eff}. Also the alpha eigenvalue (time constant) of the system is determined by a search procedure based upon successive determinations of k_{eff}.

Both the inner and outer iterations are accelerated using the diffusion synthetic method. See page 8-14 for the theory of this method.

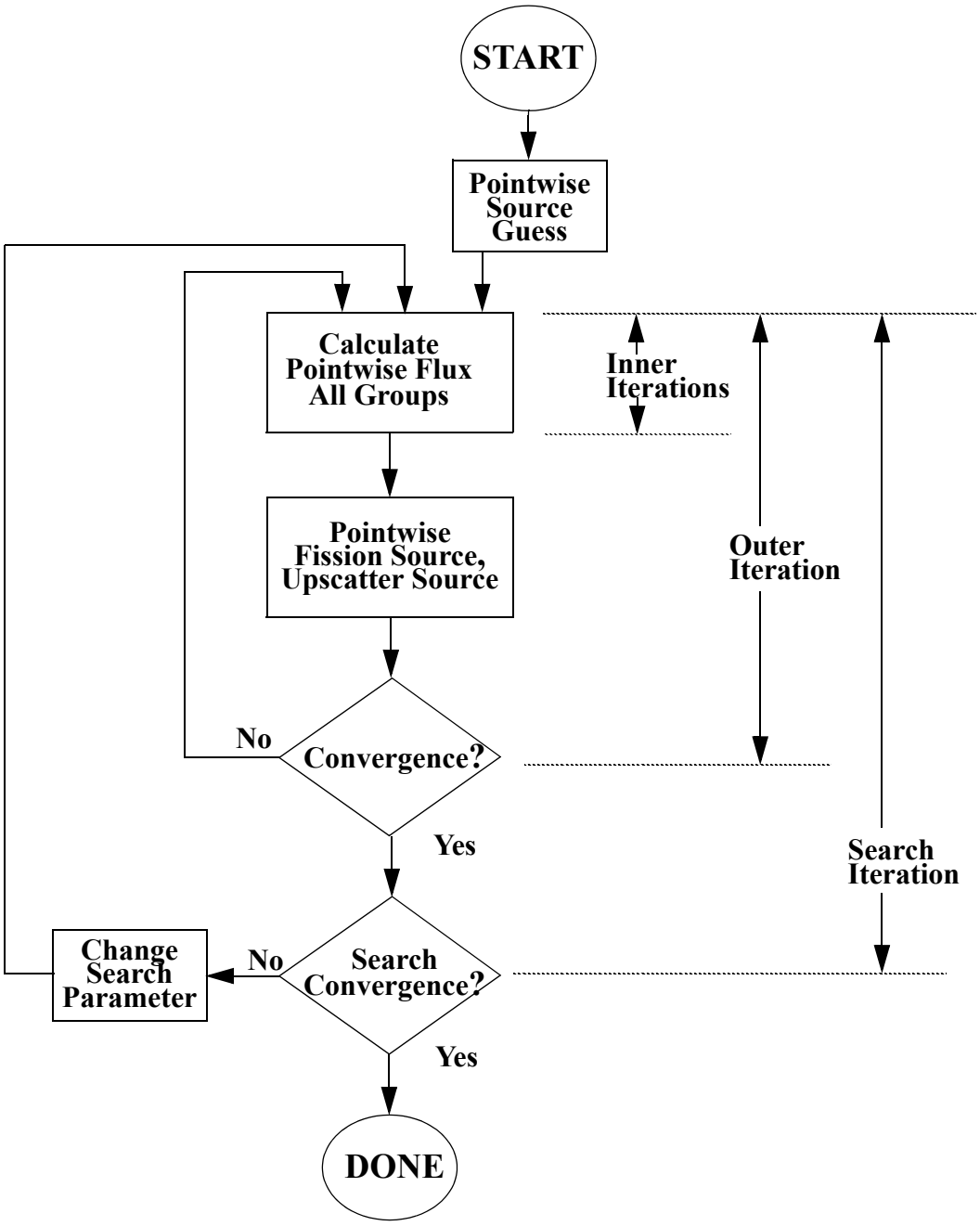

Figure 1.2 Simplified flow diagram of SOLVER iteration strategy

Modular Structure and Interface Files

There are some times when the user must be aware that the code is constructed on a modular basis with files supplying the communication between modules. This general structure is shown in Figure 1.3. Each of the solution techniques employs a different solver module.

The purpose of the input module is to convert the text input into interface files that then drive the solver and optionally the edit modules.

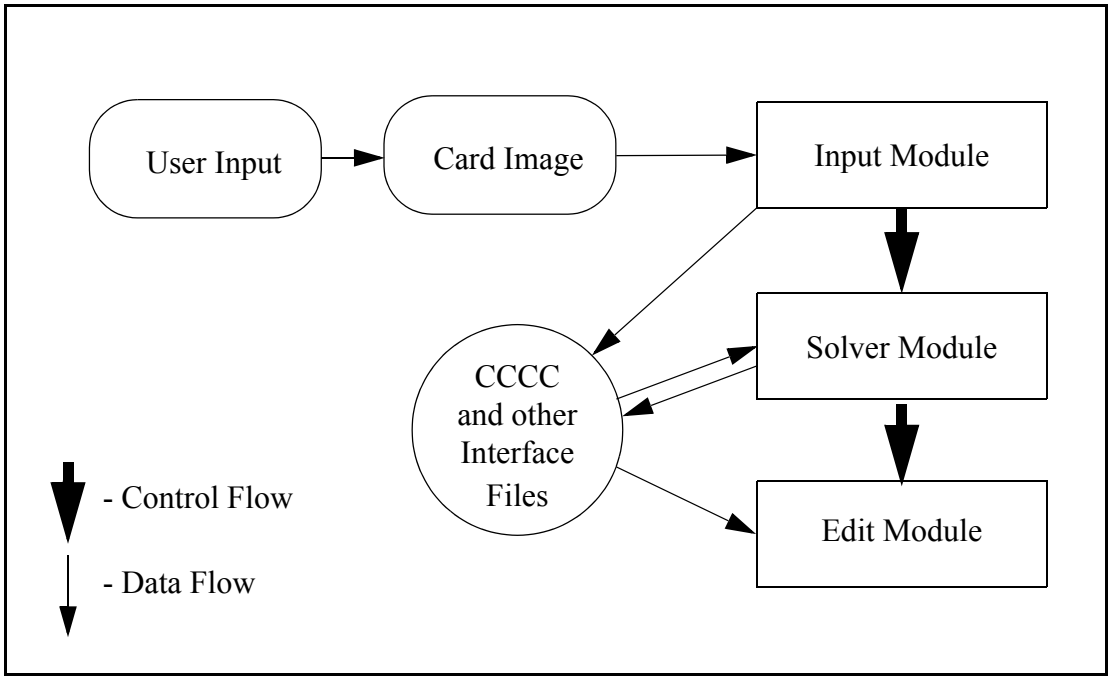

Figure 1.3 PARTISN Structure

More detail on this topic will be found in the chapter “PARTISN —CODE STRUCTURE”.

REFERENCES

1. R. E. Alcouffe, R. S. Baker, F. W. Brinkley, D. R. Marr, R. D. O'Dell, and W. F. Walters, "DANTSYS: A Diffusion Accelerated Neutral Particle Transport Code System," Los Alamos National Laboratory Manual LA-12969-M (June 1995)